

Solving Protein Structures using In-house X-ray Systems: Experiences with SAD Phasing

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Recent advances in hardware and software tools have made it easier to obtain de novo structural information in the home lab. Single-wavelength anomalous diffraction (SAD) techniques with Cu radiation are now widely used for structure solution even in cases involving weak scatterers. The anomalous signal can also provide assistance when using other techniques such as molecular replacement and model refinement. Brighter and more stable x-ray sources combined with high sensitivity, low noise CCD detectors have greatly improved the quality of data collected in-house. This is critical for determining phasing information away from the absorption edge of the anomalous scatters. Improvements in software have also increased success rates for SAD phasing experiments. Recently, a feature has been incorporated in SHELXE, which combines a main-chain trace together with density modification to help improve noisy electron density maps. Phases calculated from the traced residues are combined with the initial estimates to help in cases where the starting phases are poor. Examples of protein structure determination by SAD phasing using the SHELX suite will be discussed.